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High Production Volume (HPV) Chemical Challenge Program

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Data Review and Test Plan for Allyl alcohol

CAS RN 107-18-6

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Submitted by Lyondell Chemical Company, One Houston Center, Suite 1600, 1221 McKinney Street, Houston, TX, 77010

Allyl Alcohol (CAS RN 107-18-6)
High Production Volume (HPV) Chemical Challenge
Data Review and Test Plan

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Plain English Summary

This document reviews the data availability for the EPA High Production Volume (HPV) chemical endpoints (physical-chemical properties, environmental fate and pathways, ecotoxicity and human/mammalian health effects) and provides a proposed test plan for allyl alcohol (CAS Registry Number 107-18-6). Allyl alcohol is an intermediate chemical used primarily in the manufacture of other chemicals.

There is adequate information available for allyl alcohol to meet the HPV Chemical Challenge requirements for physical-chemical and environmental fate and pathway data, acute toxicity to fish, and the human/mammalian health endpoints of acute toxicity, repeated dose toxicity, reproductive toxicity (fertility) and genetic toxicity. To complete the HPV Chemical Challenge Program requirements for allyl alcohol testing is proposed to characterize acute toxicity on aquatic plants and invertebrates and effects on mammalian embryo-fetal development and teratogenicity.

Test Plan

Allyl Alcohol **CAS RN: 107-18-6**		Information	OECD Study	GLP	Other Study	Estimation Method	Acceptable	Testing Required
STUDY		**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**	**Y/N**
PHYSICAL - CHEMICAL DATA								
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapor Pressure	Y	N	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	Y	N	Y	N
2.6	Water Solubility	Y	N	N	Y	N	Y	N
ENVIRONMENTAL FATE AND PATHWAYS								
3.1.1	Photodegradation	Y	N	N	Y	N	Y	N
3.1.2	Stability in Water	Y	N	N	N	N	Y	N
3.4	Transport and Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	N	N	N	Y	Y	N
ECOTOXICOLOGICAL DATA								
4.1	Acute Toxicity to Fish	Y	N	N	Y	N	Y	N
4.2	Toxicity to Daphnia	Y	N	N	Y	N	N	**Y**[1]
4.3	Acute Toxicity to Algae	N	N	N	N	N	N	**Y**[2]
TOXICOLOGICAL DATA								
5.1	Acute Toxicity	Y	N	N	Y	N	Y	N
5.4	Repeated Dose Toxicity	Y	N	N	Y	N	Y	N
5.5	Genotoxicity *In Vitro* (Bacterial Test)	Y	N	N	Y	N	Y	N
5.6	Genotoxicity *In Vivo*	Y	N	Y	Y	N	Y	N
5.8	Reproductive Toxicity	Y	N	N	Y	N	Y	N
5.9	Development Toxicity / Teratogenicity	Y	N	N	Y	N	N	**Y**[3]

[1] OECD 202
[2] OECD 201
[3] OECD 414

1. Introduction

This Data Review and Test Plan and accompanying Robust Summaries for allyl alcohol (CAS RN 107-18-6) were prepared by Lyondell Chemical Company (Lyondell) to meet its commitments under the United States Environmental Protection Agency HPV Challenge Program.

The purpose of this document is to identify and summarize key studies describing physical-chemical properties, environmental fate, ecotoxicity and mammalian/human health effects in a manner consistent with the requirements of the HPV Chemical Challenge endpoints (equivalent to OECD SIDS Level 1 data package).

Table 1. General Substance Information (Identify)

Common Name	Allyl Alcohol
CAS No.	107-18-6
Molecular Formula:	C_3H_6O
Structural Formula:	$CH_2=CHCH_2OH$
Molecular Weight:	58.08
Physical state:	Liquid
Synonyms:	2-propen-1-ol; 1-propenol-3; vinyl carbinol

2. Production and Use

2.1 Production

Allyl alcohol (CAS 107-18-6) is an intermediate chemical manufactured by Lyondell Chemical Company at sites in the United States and The Netherlands. Projected global production is estimated at 175 million pounds. Approximately 140 million pounds will be used captively by Lyondell for manufacture of downstream derivatives.

Allyl alcohol is also produced in Asia mainly by two Japanese producers, Showa Denka and Daicel. Estimated total Asian production is about 125 million pounds.

2.2 Use

Allyl alcohol is a bifunctional molecule used by chemical manufacturers for a multitude of purposes by reaction of the alkene functionality, the hydroxy functionality, or both.

A significant use for allyl alcohol is as an intermediate in the production of 1,4-Butanediol (CAS RN 110-63-4) and 2-Methyl-1,3-Propanediol (CAS RN 2163-42-0). Other commercial uses of allyl alcohol include manufacture of allyl diglycol

carbonate (CAS RN 142-22-3), used in optical resins; allyl glycidyl ether (CAS RN 106-92-3) used as silane coupling agents for a multitude of applications, such as water treatment and glass adhesion, diallyl phthalate (CAS RN 131-17-9), which may be used as a plasticizer, and allyl methacrylate (CAS RN 96-05-9) and styrene allyl alcohol (CAS RN 25119-62-4) resins for coatings applications.

3. Evaluation of OECD SIDS Endpoints

3.1. Physical-Chemical Data

Adequate information is available from handbooks and other published sources to characterize the physical-chemical properties of allyl alcohol:

Table 2. Physical-Chemical Data

Property	Value	Rel †	Source
Melting point	-129 ºC	2	Howard (1989); JETOC (1992); Verschueren (1996)
Boiling point	96.9 ºC	2	Verschueren (1996)
	97 ºC		Weast and Astle (1985)
Relative density	0.825	2	Verschueren (1996)
	0.854		Windholz et al. (1983) Weast and Astle (1985)
Vapor pressure	20 mmHg, 20ºC	2	Verschueren (1996)
	23.5 mm Hg, 25ºC		Howard (1989)
	23.8mm Hg 25ºC		Weast and Astle (1985)
	26.1mm Hg		EPI (2000)
Water solubility	1E+006 g/m^3	2	EPI (2000)
	Forms constant boiling mixture, 72.3% allyl alcohol:27.7% water		Windholz et al. (1983)
Log K_{ow}	0.17	2	Howard (1989); Sangster (1989); Verschueren (1996)
	-0.25		Lipnick et al. (1987)

† Reliability according to Klimisch criteria.

Conclusion: Adequate information is available to characterize all physical-chemical endpoints. No testing is proposed.

3.2. Environmental Fate and Pathways

A calculated half-life of 7.44 hr ($1x10^6$ OH/cm^3) and rate constant of $2.59x10^{-11}$ cm^3/molecule-sec has been obtained for reaction of allyl alcohol with hydroxyradicals in air (Grosjean et al. (1993a), Rel 2). Reaction with ozone yields a removal half-life of 5.52 hours (100 ppb ozone) (Grosjean et al. (1993a), Rel 2) with formaldehyde, hydroxyacetaldehyde and a monofunctional carbonyl moiety formed as reaction products (Grossjean et al. (1993b), Rel 2). Approximately one third of an initial concentration of allyl alcohol (100 ppm) was converted to CO_2 and CO following 2 hours irradiation at wavelengths of 230-300 nm, indicating some potential for photolytic degradation (Hustert and Parlar (1981), Rel 2).

Allyl alcohol contains no groups susceptible to hydrolysis.

Results of MacKay Level I modeling indicate that environmental releases will partition mainly to water (Armstrong (2003a), Rel 2). Results from the Level III program indicate releases to air would remain in the air, releases to water will remain in water, and releases to soil are likely to remain in soil (Armstrong (2003a), Rel 2).

While no guideline biodegradation studies were located, handbook data report that aerobic removal exceeds 82-86% of theoretical BOD after 2-3 weeks (Howard (1989), Rel 2; JETOC (1992), Rel 2). A BOD of 1.6 to 1.8 g/g (Heukelekian and Rand (1955), Rel 2; Bridie et al. (1979a), Rel 2) and a ThOD of 2.21 g/g (Bridie et al. (1979a), Rel 2) indicate that allyl alcohol is readily biodegradable.

No measured BCF data were located, however log P_{ow} values of –0.25 and 0.17 (see Section 2.1) and a predicted BCF of 3.16 (from BCFWin model; Armstrong (2003b), Rel 2) indicate that it is not likely to bioaccumulate in biological systems.

Conclusion: Adequate information is available to characterize all environmental endpoints. No testing is proposed.

3.3 Ecotoxicological Data

No results are available from guideline ecotoxicity studies, however other data were found that support a preliminary assessment of the effects of allyl alcohol on fish and invertebrates.

Table 3. Ecotoxicological Data

	Result	Rel †	Source
Fish, 96 hr LC_{50}	0.32 mg/l	2	Ewell et al. (1986)
Fish, 24 hr LC_{50}	approx. 1 mg/l	2	Bridie et al. (1979b)
Daphnia, 96 hr EC_{50}	0.25-0.4 mg/l	2	Ewell et al. (1986)
Alga	no data	--	

† Reliability according to Klimisch criteria.

Ewell et al. (1986) reported results from a multi-species exposure system that allowed the simultaneous exposure of seven freshwater organisms (pillbug, water flea, flatworm, sideswimmer, snail, segmented worm, fathead minnow) to various concentrations of allyl alcohol. This returned a 96 hr LC_{50} of 0.32 mg/l for *Pimephales promelas* (fathead minnow) and a 96 hr EC_{50} of 0.25-0.4 mg/l for *Daphnia magna* (water flea). Other results are in broad agreement, with a 24 hr LC_{50} of approx. 1 mg/l for *Carassius auratus* (goldfish) (Bridie et al. (1979), Rel 2). No data were located on the potential acute effects of allyl alcohol on aquatic plants.

Conclusion: Results from non-standard tests provide consistent results which indicate that allyl alcohol is very toxic toward fish, with a $LC_{50} \leq 1$ mg/l; no further testing is therefore proposed for aquatic vertebrates. The EC_{50} for invertebrates is of a similar order however only a single result, obtained using a novel (mixed) test system, was located. A guideline study using *Daphnia magna* is proposed to confirm this value. In the absence of any information on effects on aquatic plants, a guideline acute algal toxicity test is also recommended.

3.4 Toxicological Data

3.4.1 Acute toxicity

Adequate data are available for an assessment of the acute toxicity of allyl alcohol in animals after inhalation, ingestion and skin contact. Data are also available on skin and eye irritation potential (non-SIDS endpoints).

Table 4. Acute Toxicity Data

Route	Species	Result	Comment	Rel †	Source
Inhalation LC_{50}	Rat	125-140 ppm	4 hr exposure	2	Dunlap et al. (1958)
Oral LD_{50}	Rat	70 mg/kg bw		2	Jenner et al. (1964)
	Rat	99-105 mg/kg bw			Dunlap et al. (1958)
	Mouse	96 mg/kg bw			Smyth and Carpenter (1948)
Dermal LD_{50}	Rabbit	89 mg/kg		2	Dunlap et al. (1958)
Skin irritation	Rabbit	slightly irritating	24 hr, occlusion	2	Dunlap et al. (1958)

Eye irritation	Rabbit	irritating	erythema, chemosis and corneal opacity at 24 hr, reversible	1,2	Jacobs and Martens, 1989; Dunlap et al. (1958)

† Reliability according to Klimisch criteria.

3.4.2. Repeated dose toxicity

Results from subchronic toxicity studies in rats provide adequate information on the consequences of repeated inhalation or oral (drinking water) exposure to allyl alcohol. Additional information on the consequences of repeated gavage exposure is also expected once results from completed NTP sub-chronic studies in rats and mice are finalized.

Dunlap et al. ((1958), Rel 2) exposed groups of male Long-Evans rats to atmospheres containing up to 150 ppm allyl alcohol for 7 hr/d, 5 d/wk for 12 wk. Clinical signs reported at the highest exposure level included severe irritation of the respiratory tract and eye, with 100% mortality after 10 exposures. Similar but less pronounced effects were present in animals exposed to 40-100 ppm. Body weight gain was significantly decreased in animals exposed to $\geq$ 20 ppm, with kidney weights increased after exposure to $\geq$ 40 ppm. Relative lung weights were also increased at $\geq$ 40 ppm (however incomplete data collection means that responses at lower concentrations were not characterized). Although pre-dating modern guidelines, these findings are consistent with a NOAEC for body weight effects of 5 ppm, and a systemic NOAEC (increased relative kidney weight) of 20 ppm.

This same author (Dunlap (1958), Rel 2) also reported results for male and female Long-Evans rats exposed to allyl alcohol via drinking water for 13 wk, at exposure concentrations up to 1000 ppm. Water intake was decreased in all treated groups in a dose-related manner, presumably reflecting unpalatability of the dosing solutions, with a calculated received intake of 67 or 72 mg/kg bw/d for high-dose females and males, respectively. Body weight gain was statistically significantly decreased in both sexes ingesting $\geq$ 500 ppm, with a dose-related increase in relative kidney wt (significant $\geq$ 250 ppm, both sexes) and relative liver weight (significant only in males $\geq$ 250 ppm). Although possible confounding effects due to decreased water intake cannot be excluded, these results are consistent with a NOAEL for organ weight changes of 11.6 mg/kg bw/d in males and 13.2 mg/kg bw/d in females given 100 ppm allyl alcohol in drinking water.

In a second ingestion study (Carpanini et al. (1978), Rel 2), Wistar rats of both sexes were allowed free access to drinking water containing 50-800 ppm allyl alcohol for up to 15 wk (equivalent to 4.8-48.2 mg/kg bwt/d for males and 6.2-58.4 mg/kg bwt/d for females). Water intake and urine concentrating ability were decreased (generally statistically significant) in treated groups in a dose-related manner, with significant reductions in body weight and food intake in males at $\geq$

200 ppm and females at 800 ppm. The majority of these findings appeared secondary to a reduction in water intake that was particularly pronounced in high dose animals. This was presumed to reflect poor palatability of the dosing solutions. Against this background, there was a more generalized increase in absolute kidney weight (females), relative kidney weight (both sexes) and relative stomach weight (both sexes) in the intermediate and high dose groups. While local irritation (stomach) or dehydration (kidney) may have contributed in part to these findings, they may also be indicative of mild systemic renal toxicity with a sub-chronic NOAEL of 50 ppm in females (equivalent to 6.2 mg/kg bwt/d) and 100 ppm in males (8.3 mg/kg bwt/d).

No-effect levels and key findings from these studies are summarized in the table below:

Table 5. Repeated Dose Toxicity Data

Route	Species	NOAEC/NOAEL	Effects	Rel	Source
Inhalation	Rat	5 ppm 20 ppm	Dec. bwt gain Inc. rel. kidney wt	2	Dunlap et al. (1958)
Oral, drinking water	Rat	11.6-13.2 mg/kg bwt/d	Inc. rel kidney Inc. rel liver wt	2	Dunlap et al. (1958)
Oral, drinking water	Rat	6.2-8.3 mg/kg bwt/d	Inc. rel. kidney wt	2	Carpanini et al. (1978)

Information on the NTP website (http://ntp-server.niehs.nih.gov/) indicates that 13 week gavage studies have been performed in male and female F344 rats (0, 1.5, 3, 6, 12 or 25 mg/kg bwt/d) and B6C3F1 mice (0, 3, 6, 12, 25 or 50 mg/kg bwt/d), however no report of the findings is currently available.

Overall, the currently available data suggest that the kidney is a potential target for allyl alcohol following repeated inhalation or ingestion. Although pre-dating modern guidelines, these studies are considered adequate to characterize the sub-chronic toxicity of allyl alcohol. Additional information will be available when results from completed NTP studies are finalized. No further testing is proposed.

3.4.3 Genetic toxicity

Results from *in vitro* genotoxicity tests in bacterial systems present inconsistent results. A positive response was reported in *Salmonella typhimurium* TA1535 in a liquid preincubation assay in the presence of hamster S9 (negative with rat S9 and/or with plate incorporation) (Lijinsky and Andrews (1980), Rel 2), and in TA100 using liquid preincubation in the absence of S9 (weaker response in presence of S9, source not specified) (Lutz et al. (1983), Rel 2. While metabolism to acrolein by mammalian (or bacterial) alcohol dehydrogenases may explain these findings (see Section 3.4.6.), other studies (NTP (unpublished results), Rel 2) found no

evidence of mutagenic activity when either stain was tested using a liquid preincubation protocol in the presence and absence of rat or hamster S9. Other limited data suggests that allyl alcohol may induce mutations in mammalian V79 cells *in vitro*, as assessed from induction of resistance to 6-thioguanine (Smith et al. (1990), Rel 4).

In contrast to the above findings *in vitro*, results from *in vivo* studies performed by NTP ((unpublished data), Rel 2) show that it does not induce micronuclei in rat femoral bone marrow (no effect up to the limit of toxicity) or mouse blood (inactive following sub-chronic treatment). It also failed to induce dominant lethal effects in male SD rats given 25 mg/kg bw by gavage (equivalent to approx. one quarter to one third of the LD50; see Section 3.4.1) for 11 wk prior to mating with untreated females (Jenkinson and Anderson (1990), Rel 2).

Table 6. Genetic Toxicity Data

End point	Test system	Conditions	Result	Rel	Source
in vitro					
Gene mutation	Bacterial cells	TA 98, 100, 1535, 1537, 1538; liquid preincubation, hamster S9	Positive in TA1535 with S9	2	Lijinsky and Andrews (1987)
		TA 100, liquid preincubation, rat S9	Positive in TA100 without S9 (weak response +S9)	2	Lutz et al (1982)
		TA 100, 1535, 97, 98; liquid preincubation, rat and hamster S9	Negative	2	NTP (unpublished results)
	Mammalian cells	V79 cells (6-thioguanine resistance)	Positive	2	Smith et al. (1990)
Chromosomal aberrations	--	--	--	--	--
in vivo					
Micronuclei	Bone marrow, F-344 rat	≤ 20 mg/kg bwt/d, i.p., 3 consecutive days	Negative (higher doses precluded by mortality)	2	NTP (unpublished results)
Micronuclei	Blood, B6C3F1 mouse	≤ 50 mg/kg bwt/d, gavage, 13 wk	Negative	2	NTP (unpublished results)
Dominant lethal	SD rat	25 mg/kg, 33 wk	Negative	2	Jenkinson and Anderson, (1990)

3.4.4 Carcinogenicity (non-SIDS endpoint)

There was no increase in tumors in male and female F344 rats administered allyl alcohol in drinking water (300 mg/l) for 106 wk, followed by observation until natural death (wk 123-132) (Lijinsky and Reuber (1987), Rel 2). Although small group sizes and use of a single dose level limit the overall reliability of these findings, the treatment level compares favorably with the 50-100 ppm NOAEC obtained from sub-chronic drinking water studies and the study is considered supportive of this assessment.

3.4.5 Reproductive and Developmental toxicity

3.4.5.1 Reproductive toxicity

While no guideline reproductive toxicity test results are available, no adverse histopathological changes were detected in testis, ovary or uterus from Wistar rats given up to 800 ppm allyl alcohol in drinking for 15 weeks (equivalent to a top dose of 48.2 or 58.4 mg/kg bwt/d in males and females, respectively) (Carpanini et al. (1978), Rel 2). Total sperm count, epididymal sperm concentrations and fertility were unaltered in SD rats given 25 mg/kg bwt for 11-15 wk as part of a male dominant lethal assay (Jenkinson and Anderson (1990), Rel 2). Additional information on gonad weight weights and histopathology, together with data on sperm quality and vaginal cytology, are anticipated when results from an NTP 13 week study are finalized (NTP (unpublished results)).

3.4.5.2 Developmental toxicity / Teratogenicity

No relevant studies were located on the potential effects of allyl alcohol on embryo-fetal development.

3.4.6. Metabolism (non-SIDS endpoint)

Extensive necrosis and covalent binding of radiolabel was observed in the periportal region of the liver in male SD rats given 14C-allyl alcohol by i.p. injection, whereas no necrosis and an 80% reduction in covalent binding was apparent in animals pre-treated with pyrazole (Reid (1972), Rel 2). These findings are compatible with decreased toxicity after inhibition of alcohol dehydrogenase activity *in vivo*. In other studies (Patel et al. (1983), Rel 2), greater hepatic necrosis, elevated levels of plasma GPT and greater covalent binding to liver protein was noted in SD rats given ^{14}C-allyl alcohol compared with rats given an equivalent dose of deuterated allyl alcohol. This reduction in toxicity presumably corresponds with slower activation of the deuterated substrate by alcohol dehydrogenase (steric hindrance). *In vitro* studies showed significantly greater formation of acrolein and acrylic acid by liver fractions when ^{14}C-allyl alcohol was substrate compared to that seen in incubations containing deuterated allyl alcohol (Patel et al. (1983), Rel 2). These NADH-dependent reactions were sensitive to inhibition by pyrazole and

disulfuram, indicating a role for alcohol- and aldehyde dehydrogenases in the hepatic metabolism of allyl alcohol.

Overall these observations suggest that alcohol- and aldehyde dehydrogenases contribute to the toxicity of allyl alcohol *in vivo*.

Conclusion: Adequate data exist to demonstrate that allyl alcohol is acutely toxic after ingestion, inhalation or skin contact, while results from sub-chronic studies (inhalation, ingestion) provide evidence of potential effects on the kidney, with a NOAEC of 20 ppm and a NOAEL of 6-8 mg/kg bwt/d. Additional information on repeat dose effects is also expected once results from completed NTP gavage studies in rats and mice are published. The SIDS requirements for acute and repeat dose toxicity are therefore met, and no further testing is proposed.

Results from *in vitro* genotoxicity tests are inconsistent with some studies indicating that allyl alcohol causes gene mutations in bacterial and mammalian cells *in vitro*, while others (using identical test conditions) were negative. While metabolism to acrolein and acrylic acid by alcohol- and aldehyde dehydrogenases may explain these positive findings, results from *in vivo* studies are consistently negative, with no increase in micronuclei in rat femoral bone marrow or mouse blood and no effect on male-mediated dominant lethality. These findings are consistent with efficient detoxication of allyl alcohol and its metabolites *in vivo*.

Results from a sub-chronic drinking water study demonstrate no adverse effect on gonadal histology in male and female rats given allyl alcohol at received doses of 48 or 58 mg/kg bwt/d, respectively, for 15 wk. Additional information on gonad histopathology, sperm quality and vaginal cytology is expected once results from an NTP 13 week study are finalized. There was no functional impact on sperm quality or fertility in male rats given 25 mg/kg bwt/d allyl alcohol for 11-15 wk as part of a dominant lethal investigation. Overall, the SIDS requirement for information on reproductive (fertility) effects is met and no further testing is proposed.

No relevant data were located on potential effects of allyl alcohol on embryo-fetal development. Further testing is proposed for this endpoint.

4. Summary and Conclusion

There is adequate information available for allyl alcohol to meet the HPV Chemical Challenge requirements for physical-chemical and environmental fate and pathway data, acute toxicity to fish, and the human health endpoints of acute toxicity, repeated dose toxicity, and genetoxic toxicity, and reproductive toxicity.

To complete the HPV Chemical Challenge Program requirements for allyl alcohol, testing is proposed on aquatic species (OECD TG 201, “Alga, growth inhibition test”; OECD TG 202, “*Daphnia* sp. acute immobilization test and reproduction

test”) and on mammalian embryo-fetal development and teratogenicity (OECD TG 414, “Prenatal developmental toxicity study”).

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